Supporting information

The impact of organic nitrates on summer ozone formation in Shanghai, China

Li et al.,

S1. The description of mechanistic uptake in Zare Mechanism

Firstly, the BVOCs oxidized by OH and NO_3 have been refined and supplemented, and the various reactions between RO_2 and NO, as well as the conversion between ROx, have been updated to ensure the applicability in high/low NO_x environments (Zare et al., 2018). For isoprene, the mechanism update contains refinements for oxidation reactions initiated by OH and NO_3. For monoterpenes, the relevant updates mainly include reaction rate constants for API and NO_3 and API is represented by α-pinene and β-pinene. Under the above updates, ANs contain a total of 24 species, of which 4 are secondarily generated. For the deposition, except the deposition rates of R_4NO (C4 nitrooxycarbonyl hydroperoxide), PROPNN (propanone nitrate), and TONIH (C10 nitrooxy hydroperoxide) were set to 1.3±0.6, 1.7±0.6 and 0.8±0.4 cm/s, respectively, the rest were set to 1.5 cm/s according to ISOPN (hydroxy isoprene nitrates) (Nguyen et al., 2015). The uptake of ANs was quantified by speciation parameterization, and key parameters mainly included uptake coefficients, aerosol surface areas, and molecular motion rates. The uptake coefficients are distributed in the range of 0.005 - 0.01 according to the ANs species, the molecular speed is valued by ISO, and the aerosol surface area concentration is parameterized according to the empirical formula through the mass concentration of $PM_{2.5}$ (Wang et al., 2021).
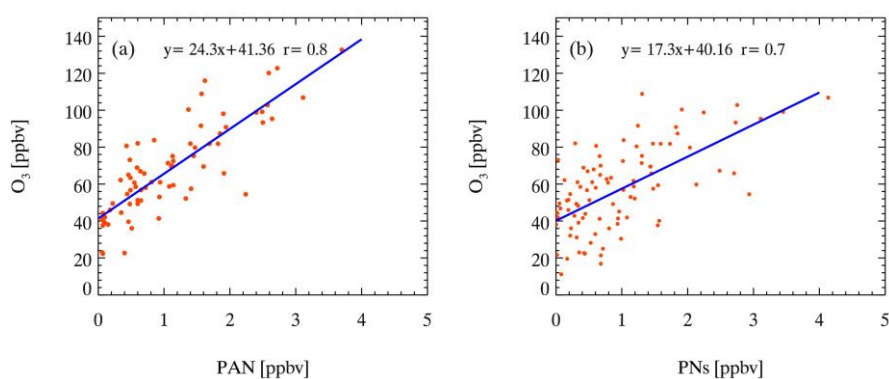
Figure S1. Correlation analyses of ozone and PAN (a) or PNs (B) during the Shanghai campaign.
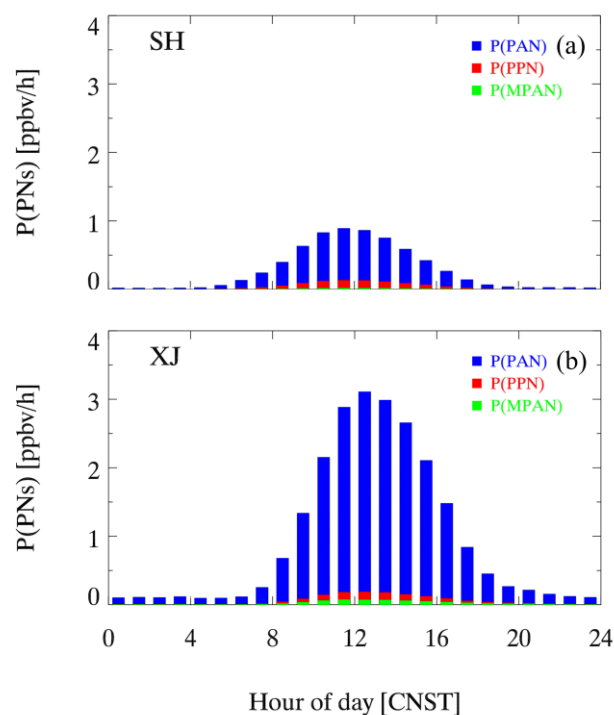
Figure S2. The mean diurnal production rate of PNs (P(PNs)) calculated by kinetic calculation method during Shanghai campaign (a) and Shanghai campaign (b). The kinetic calculation method is to calculate the total production potential of PAN, MPAN and PPN, which is determined by VOCs distribution, reaction rate constant and OH concentration, detailed in previous study (Li et al., 2023).

Table 1. The species of ANs precursors observed during the Shanghai campaign with corresponding branching ratio and averages of concentration (ppbv).

Species	Branching ratio	Concentration
ethane	0.019	2.858
propane	0.036	2.388
n_butane	0.077	1.115
n_pentane	0.105	0.384
iso_butane	0.096	0.851
iso_Pentane	0.007	0.522
_2_2_Dimethylbutane	0.152	0.016
cyclopentane	0.045	0.110
_2_Methylpentane	0.097	0.086
_3_Methylpentane	0.109	0.113
_2_2_4_trimethylpentane	0.14	0.028
methylcyclopentane	0.14	0.096
n_hexane	0.141	1.052
Cyclohexane	0.16	0.144

methylcyclohexane	0.17	0.048
n_heptane	0.178	0.133
n_octane	0.226	0.072
n_nonane	0.393	0.033
n_decane	0.417	0.035
ethene	0.0086	1.169
propene	0.015	0.258
_1_butene	0.025	0.077
_2_methyl_1_butene	0.02	0.009
_3_methyl_1_butene	0.059	0.002
_2_methyl_2_butene	0.034	0.004
trans_2_butene	0.034	0.049
cis_2_butene	0.034	0.104
_1_pentene	0.059	0.022
trans_2_pentene	0.064	0.012
cis_2_pentene	0.064	0.017
_1_3_butadiene	0.007	0.018
_1_hexene	0.055	0.010
isoprene	0.07	0.154
methacrolein	0.15	0.069
methyl_vinyl_ketone	0.11	0.144
ALPHA_PINENE	0.18	0.008
BETA_PINENE	0.24	0.015
D_LIMONENE	0.23	0.010
Benzene	0.034	0.235
p_diethylbenzene	0.093	0.017
toluene	0.029	0.634
o_Ethyltoluene	0.106	0.014
m_Ethyltoluene	0.094	0.015
p_Ethyltoluene	0.137	0.009
o_xylene	0.081	0.139
M_P_xylenes	0.074	0.311
ethylbenzene	0.072	0.190
_1_3_5_trimethylbenzene	0.081	0.008
_1_2_4_trimethylbenzene	0.105	0.021
_1_2_3_trimethylbenzene	0.119	0.011
iso_propylbenzene	0.11	0.010
Weighting averages	0.053	/

References

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